VIII.1 Hydrogen Safety, Codes and Standards R&D – Release Behavior

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Start Date: Fiscal Year (FY) 2002
End Date: Project continuation and direction determined annually by DOE

FY 2011 Objectives

(1) Scenario Analysis, Risk Assessments for Safety
- Develop a scientific basis and the associated technical data for modifying or developing new codes and standards for the commercial use of hydrogen.
- Develop benchmark experiments and a defensible analysis strategy for risk assessment of hydrogen systems.
- Develop and apply risk-informed decision-making tools in the codes and standards development process.

(2) Hazards Mitigation Technologies for Hydrogen Applications
- Determine the effectiveness of ventilation, active sensing, and similar engineered safety features.

(3) Codes and Standards Advocacy
- Provide technical management and support for the Safety, Codes and Standards sub-program element.
- Participate in the hydrogen codes and standards development/change process.

Technical Barriers

This project addresses technical barriers from the Codes and Standards section of the Fuel Cell Technologies 2007 Multi-Year Research Plan:

(F) Limited DOE Role in the Development of International Standards
(I) Conflicts Between Domestic and International Standards
(N) Insufficient Technical Data to Revise Standards
(P) Large Footprint Requirements for Hydrogen Fueling Stations
(Q) Parking and Other Access Restrictions

Contribution to Achievement of DOE Codes and Standards Milestones

This project will contribute to achievement of the following DOE milestones from the Codes and Standards section of the Fuel Cell Technologies Program Multi-Year Research, Development and Demonstration Plan:

- **Milestone 21**: Completion of necessary codes and standards needed for the early commercialization and market entry of hydrogen energy technologies. (4Q, 2012)
- **Milestone 8**: Complete investigation of safe refueling protocols for high pressure systems. (1Q, 2012)
- **Milestone 9**: Complete risk mitigation analysis for advanced transportation infrastructure systems. (1Q, 2015)
- **Milestone 12**: Complete research needed to fill data gaps on hydrogen properties and behaviors. (2Q, 2010)

FY 2011 Accomplishments

- Improved hydrogen jet release and ignition understanding with high-fidelity data.
- Measured dispersion statistics and ignition probability boundaries for a high source pressure release with a choked exit flow and compared measurements to predicted values.
- Acquired and analyzed hydrogen release data into vehicle compartments in support of a new Global Technical Regulation in support of a performance-based test methodology for hydrogen powered vehicles.
- Key validation experiments of H_2 releases and delayed ignition deflagration have been performed for indoor hydrogen forklift trucks.
- A consequence model for indoor releases from hydrogen forklift trucks has been developed and validated with experimental data.
- The Sandia turbulent entrainment model for cold hydrogen jets has been validated against high-momentum jet data (from Forschungszentrum Karlsruhe tests) and used in a liquid hydrogen separation distance study for National Fire Protection Association (NFPA) 2.

Introduction

The purpose of this project is to enable risk-informed development of codes and standards for hydrogen fuel cell technology that is based on a traceable, scientific foundation. Our scenario analysis and risk assessment efforts focus on defining scenarios for the unintended release of hydrogen and quantifying the consequences through scientific experimentation and modeling. Quantitative risk assessment (QRA) is used to identify risk drivers and risk mitigation strategies for the commercial use of hydrogen. We combine our validated models with QRA to support risk-informed decision-making in the code development process.

Approach

We develop an understanding of combustion behavior and thermal effects from the unintended releases of hydrogen in the built environment. We consider ignition characteristics, partially confined spaces such as hydrogen forklift trucks in warehouses, and liquid hydrogen handling. Technical information is disseminated through a variety of public channels and is used by codes and standards developers writing for the International Code Council and NFPA. International partnerships for vetting technical data and analysis methods occur through activities such as International Energy Agency Task 31 on Hydrogen Safety. Efforts in FY 2011 have focused on developing the basis for regulations and codes and standards development in the area of hydrogen releases in enclosures, ignition mechanisms, and liquefied hydrogen release behavior.

Results

Fundamental Ignition Phenomena of Unintended Hydrogen Releases

Ignition boundaries for turbulent natural gas jets have previously been found to correlate well with the flammability factor (FF), or the integration of the probability density function (PDF) between the fuel flammability limits. Although the FF does not predict flame light-up probability, it nonetheless allows modelers to determine the likelihood that an ignition kernel will form within a jet region when an ignition source is present. To verify the FF concept applies to hydrogen releases, light-up boundary, ignition probability, and concentration statistics for turbulent hydrogen jets were quantified at Sandia during FY 2008 through a combination of laser spark ignition and planar laser Raleigh scatter (PLRS) imaging. These measurements were also performed for methane jets, and it was found that the methane jet maximum axial and radial extents of the light-up boundaries were roughly a third lower. It should be noted, however, that smaller jet exit diameters and Reynolds number used for the Sandia study may have impacted the light-up flow features. An additional discrepancy, however, was that the centerline measured FF did not agree well with the measured laser spark ignition probability in the jet far field. Thus, it was concluded that the experimental methodology needed to be refined.

New ignition probability and jet light-up boundary measurements were performed in FY 2011 with the following experimental modifications: (1) the sample size was doubled; (2) a longer stabilization time was between sparks was used; (3) the number of thermocouples used to detect ignition was increased from 3 to 10; and (4) air conditioner vents and wind tunnel outlets were blocked to minimize air current disruptions. With these improvements, the new ignition probability measurements had much better agreement with the previously recorded methane and methane jet FF values, as can be seen in Figure 1. Nonetheless, methane and hydrogen light up boundaries, were essentially unchanged from the previous literature measurements; thus it was concluded the differences in flame light-up boundary were primarily driven by flow characteristics. Future measurements will quantify the jet flow features during ignition to support the engineering model development of sustained light-up phenomena.

Modeling of High Source Pressure Releases

Self-similar behavior for turbulent, subsonic heterogeneous jets exists for a broad range of gases, including hydrogen, which allows jet behavior to easily be modeled using canonical analytic expressions. However, for releases from storage pressures above the critical ratio (~1.9 for hydrogen), the exit flow chokes and underexpanded jets form, which are characterized by complex shock structure and nonuniform velocity distributions. A Mach disk at the end of the shock structure serves as the supersonic/subsonic boundary and is used as the effective source for the subsonic dispersion models; it

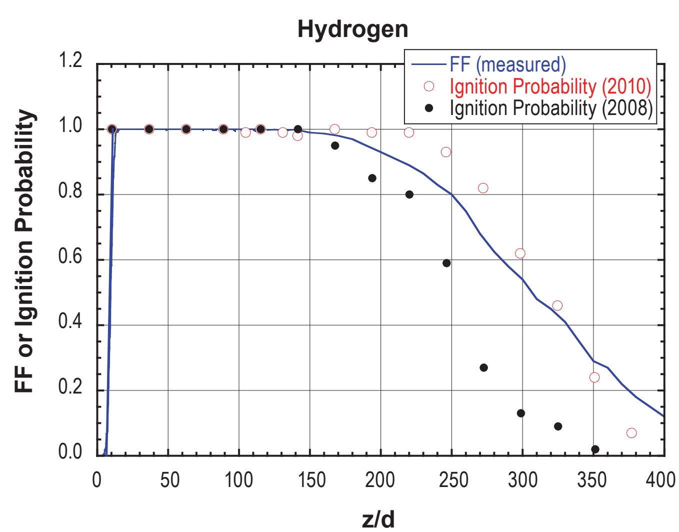
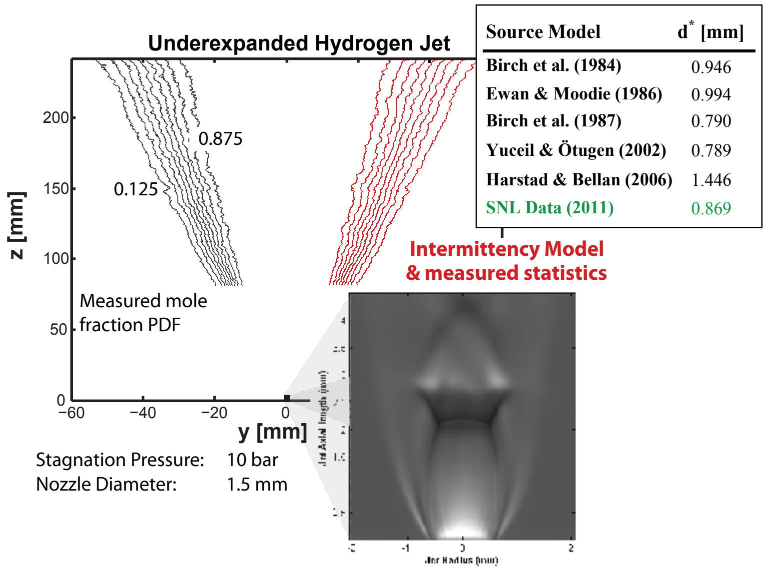


FIGURE 1. Original and Repeated Centerline Profile FF and Laser Spark Ignition Probability Measurements

is generally several factors wider than the jet exit diameter. Although source models that predict effective Mach disk diameter size and jet exit thermodynamic variables have been developed, limited validation data is available for choked hydrogen releases.

In FY 2011, the equation-of-state in these models was updated (Able-Noble) to better account for hydrogen compressibility. A new high-pressure stagnation chamber was integrated into Sandia's Turbulent Combustion Laboratory, and was used to acquire validation data from a choked hydrogen jet with a 10:1 pressure ratio and 1.5 mm nozzle diameter. The maximum measured centerline light-up distance was 367 mm downstream from the nozzle exit. Downstream concentration statistics were collected using PLRS imaging, while jet exit shock structure was imaged with schlieren photography. Measured (black) and modeled (red) FF contours from the concentration measurements are shown in Figure 2. Close agreement is achieved between the two methods, which indicate the self-similar jet behavior is preserved in the subsonic portion of the jet release. Computed effective source diameters, which are linearly proportional to ignitable boundary maximum extents, are tabulated for each model on the right. Although no model prediction was within 10% of the SNL experimental value, simpler models that neglect momentum and energy conservation performed the best while more complicated models that accounted for entropy change across the Mach disk performed the worst. More work is needed to determine why, but this is likely at least partially due to poorly predicted entrainment within the jet near field around the Mach disk. These data will ultimately be used to extend and validate the predictive capabilities of the ignition and flame light-up models and will form an important QRA input that ultimately impacts codes and standards separation distance decisions in NFPA 2, NFPA 55, and International Energy Agency 19.



Source Model	d^* [mm]
Birch et al. (1984)	0.946
Ewan & Moodie (1986)	0.994
Birch et al. (1987)	0.790
Yuceil & Ötugen (2002)	0.789
Harstad & Bellan (2006)	1.446
SNL Data (2011)	0.869

FIGURE 2. Flammability factor maps for the choked hydrogen jet ($p_0/p = 10$, d = 1.5 mm), with black contours generated from direct PDF integration, while red contours were generated from concentration statistics and an applied intermittency model. A schlieren image of jet exit shock structure is shown at the bottom, while tabulated predictions (black) and measurements (green) of the effective source diameter are shown to the right.

Performance-Based Hydrogen Leakage Testing in Passenger Vehicle Compartments

International regulatory representatives have proposed the performance-based test methodology for hydrogen fuel cell vehicle fuel system integrity certification in a new global technical regulation (GTR). For this testing methodology, automotive original equipment manufacturers (OEMs) self certify each vehicle. To ensure compliance, government regulators periodically inspect the system performance of randomly selected vehicles during barrier/rollover crash tests. Since a single failure for any safety criteria may result in a model line recall, OEMs are strongly incentivized to maintain vehicle safety compliance; however, OEMs have the flexibility to decide the design approach that best achieves the prescribed safety level. The GTR proposal specifies that the test is failed if within 1 hour post-crash, hydrogen leakage rates exceed 118 liters/min or flammable mixtures develop within the passenger cabin or trunk. An analysis of the capabilities necessary to detect the second failure mode was performed through exploratory in-vehicle leakage tests at SRI International's Corral Hallow Experimental Site. Hydrogen concentrations were primarily derived from oxygen depletion sensors, and were compared to directly measured concentrations from co-located hydrogen sensors (location details are shown in Figure 3a). Close agreement between the two sensor technologies was observed as shown in Figure 3b. Since oxygen depletion measurements have the additional advantage that nonflammable gases can be used, helium was investigated as a surrogate due to its similar diffusion and jet spreading characteristics. Good agreement in overall dispersion trends for both gases highlights the flexibility of the indirect sensor method. While hydrogen mixture fractions strongly depended on release characteristics (e.g., rate, location, type), results of an analytic examination indicate that pinhole leaks from moderate source pressures likely would produce unacceptably high in-vehicle hydrogen concentrations. The optimum sensor location for leak detection was determined to be high above the release point. Accordingly, sensor placement for crash tests involving vehicle rollovers must account for the final vehicle orientation. Test results provided quantifiable support for the U.S. National Highway Traffic Safety Administration proposal for a multinational performance-based hydrogen leakage test standard at a GTR meeting held September 8, 2010 in San Francisco, CA.

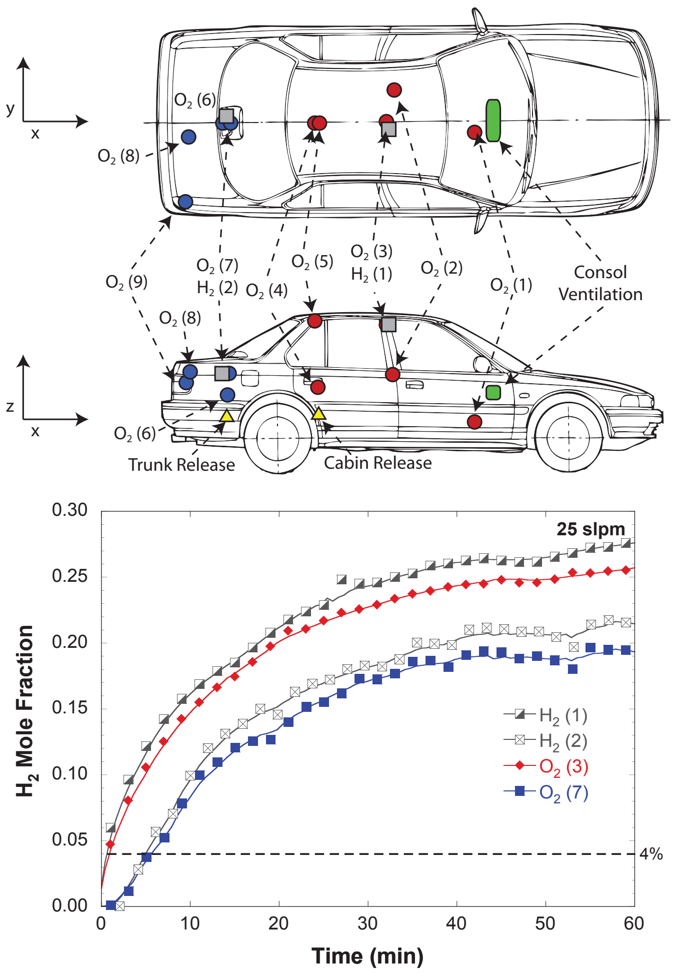


FIGURE 3. Schematic of trunk O_2 (blue), passenger cabin O_2 (red), and H_2 sensors (grey), along with ventilation (green) and release (yellow) points within the simulated fuel cell vehicle. Data shows a comparison of volumetric concentration measurements from co-located H_2 and O_2 sensors in the trunk and passenger cabin for the baseline condition.

Unintended Releases of Hydrogen in Partially Enclosed Spaces

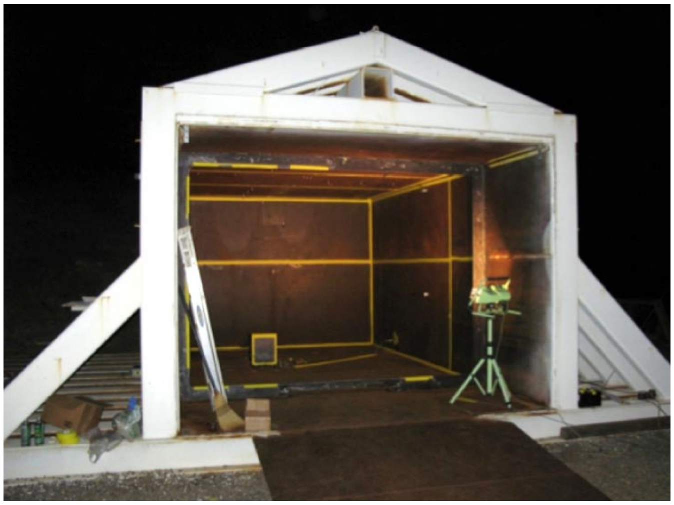
Sandia has been working with OEMs to develop scientific understanding that will form the basis for risk-informed safety codes and standards for safe operation of indoor hydrogen fuel cell forklift vehicles. A combined modeling and experimental approach has been used to develop an experimentally validated model for dispersion and ignition of unintended releases from hydrogen forklift vehicles in warehouses. As part of this work the validated forklift warehouse release model has been used to study the effect of leak size, ignition delay time, ventilation, and warehouse volume on the associated consequences. Results of this modeling study are being used in a risk analysis to develop new risk-informed indoor refueling codes and standards.

The indoor hydrogen release experiments were designed based on OEM forklift specifications and leak size, and the gaseous hydrogen indoor dispensing code in NFPA 2 and 52. The warehouse sizing, ventilation, and amount of vehicle onboard hydrogen were based on the parameters outlined in the NFPA codes. The experiments were performed in a subscale warehouse test facility (Figure 4) at the SRI Corral Hollow Experiment Site to provide data for model validation. The SRI subscale warehouse has a volume and height approximately 1/2.8 that of a full-scale 1,000 m^3 warehouse with a 7.62 m ceiling. The release diameter for the experiments was designed so that the mass flowrate matched the scaled mass flow rate versus scaled tank blow-down curve for a full-scale forklift release. Measurements were made of the hydrogen concentration, flame speed, and ignition delay overpressure in the scaled warehouse. As part of the work a dispersion model and deflagration model of the subscale warehouse and forklift geometry were developed. These models were used prior to the tests to estimate the placement of concentration and pressure sensors in the subscale warehouse and to determine the amount of expected overpressure from ignition of the hydrogen release. Pretest ignition deflagration simulations of the test geometry indicated that the maximum ignition overpressure would be approximately 30 kPa (0.3 barg) if the warehouse was completely (100%) sealed and the effects of wall heat transfer were neglected. Based on these simulations a wooden pressure relief panel was designed and placed in the doorway of the steel front wall of the scaled warehouse prior to the beginning of the deflagration testing.

Figure 4 shows comparisons of the predicted ignition overpressure from the simulations with data from the experiment for a pressure sensor in the center of the warehouse side wall nearest the forklift. Results are shown for simulations with and without heat transfer to the walls and also for the cases where the warehouse is completely sealed (100%) or the measured leakage area (36.7 cm^2) is incorporated into the model. The results with the measured air leakage rate and heat transfer to the walls are found to be in good agreement the experimental data. Figure 4 also shows that incorporating natural ventilation in the warehouse reduces the peak deflagration overpressure from approximately 25 kPa to 5 kPa.

The results of the modeling and experiments demonstrate that pressure relief panels or passive natural ventilation can be used as an effective means to mitigate deflagration overpressure arising from ignition of the released hydrogen. Simulation results also indicate that increasing the warehouse volume beyond the requirements currently specified also reduces the overpressure. Both simulations and experiments show that forced ventilation has little effect on the hydrogen concentration and deflagration overpressure in the early stages of the release.

Results of the modeling and experiments were presented to the DOE Technical Team, the Hydrogen Industrial Panel on Codes and Standards, and at the Annual Fuel Cell and Hydrogen Energy Conference. Based on feedback from these presentations a new indoor refueling task group was formed



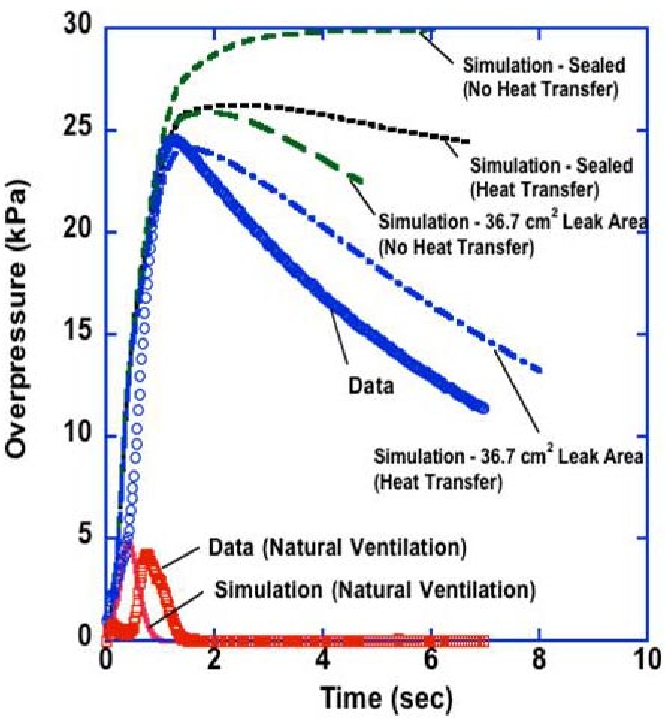


FIGURE 4. Comparison of Measured Ignition Overpressure in the SRI International Subscale Warehouse Facility with Results from FUEGO/FLACS Model Simulations

within NFPA 2 to utilize the experimental data and validated model in a science-based risk-informed process to develop new indoor refueling codes and standards for NFPA 2.

Conclusions and Future Directions

This project provides key understanding to enable the deployment of early market hydrogen systems. In FY 2011:

- We performed consequence analysis of indoor refueling and operation of hydrogen powered industrial trucks.
- Incorporated data from existing demonstration and projects into the QRA of hydrogen technologies.
- Improved the existing predictive model of ignition in turbulent flames to include sustained flame light-up probability.
- We improved the understanding of high-source pressure hydrogen releases in support of improved NFPA 2 separation distances from compressed gas applications.
- We developed an understanding of high-momentum low-temperature hydrogen plume behavior and supported NFPA 2 separation distance activities on liquid hydrogen.
- Performed risk analysis of advanced storage materials in support of NFPA 2 activities.

This project will continue to enable hydrogen and fuel cell technology deployment through developing the defensible technical basis for codes and standards. We will perform work to:

- Complete risk analysis of indoor refueling and work with codes and standards development organizations to provide technical data for science-based risk-informed indoor refueling codes and standards
- Perform study to identify potential mitigation features associated with hydrogen refueling stations and indoor refueling efforts.

FY 2011 Publications/Presentations

1. Houf, W.G., Evans, G.H., Ekoto, I., Merilo, E., and Groethe, M., "Hydrogen Releases and Ignition from Fuel-Cell Forklift Vehicles in Enclosed Spaces," 2011 Annual Fuel Cell and Hydrogen Energy Conference, Washington, D.C. Area, February 13–16, 2011.

2. Houf, W.G., and Winters, W.S., "Results from an Analytical Investigation of High Pressure Liquid Hydrogen Releases," 2011 Annual Fuel Cell and Hydrogen Energy Conference, Washington, D.C. Area, February 13–16, 2011.

3. Ekoto, I.W., Dedrick, D.E., Merilo, E., and Groethe, M., "Performance-Based Testing for Hydrogen Leakage into Passenger Vehicle Compartments," 2011 Annual Fuel Cell and Hydrogen Energy Conference, Washington, D.C. Area, February 13–16, 2011.

4. Ekoto, I.W., Merilo, E. and Groethe, M., "Hydrogen Releases and Ignition from Fuel-Cell Forklift Vehicles in Enclosed Spaces," HIPOC Meeting, Washington, D.C., February 17, 2011.

5. Houf, W.G., Evans, G., Ekoto, I., "Consequence Analysis for Unintended Hydrogen Releases within Enclosed Spaces," Combustion Research Facility News, March, 2011.

6. Houf, W.G., Evans, G., Ekoto, I., LaChance, J., Dedrick, D., Keller, J. "Hydrogen Release Behavior in Enclosures," NFPA 52 Meeting, Las Vegas, NV, Sept. 16, 2010.

7. Houf, W.G., Evans, G., James, S.C. "Unintended Hydrogen Releases in Tunnels," NFPA 52 Meeting, Las Vegas, NV, Sept. 16, 2010.

8. Houf, W.G., Evans, G., Ekoto, I., Ruggles, A., Zhang, J., LaChance, J., Dedrick D., Keller, J., "Update on Sandia Hydrogen Releases Program," IEA Task 31 Meeting, Istituto Superiore Antincendi (ISA), Rome, Italy, Oct. 4–6, 2010.

9. Houf, W. and LaChance, J., "Risk-Informed Separation Distances for Hydrogen Gas Storage Facilities," 5th Annual Hydrogen Codes and Standards Conference, NextEnergy Center, Detroit, MI, Sept. 21, 2010.

10. Houf, W.G., Evans, G.H., Ekoto, I., Merilo, E. and Groethe, M., "Hydrogen Releases and Ignition from Fuel-Cell Forklift Vehicles in Enclosed Spaces," 4th International Conference on Hydrogen Safety, San Francisco, CA, Sept. 12–14, 2011.

11. Houf, W.G. and Winters, W.S., "Simulation of High Pressure Liquid Hydrogen Releases," 4th International Conference on Hydrogen Safety, San Francisco, CA, Sept. 12–14, 2011.

12. Ekoto, I.W., Merilo, E.G., Houf, W.G., Evans, G.H., Groethe, M.A., "Hydrogen Fuel-Cell Forklift Vehicle Releases in Enclosed Spaces," 4th International Conference on Hydrogen Safety, San Francisco, CA, Sept. 12–14, 2011.

13. Merilo, E., Groethe, M., Adamo, R., Schefer, R., Houf, W., Dedrick, D., "Self-Ignition of Hydrogen Jet Fires by Electrification of Entrained Particulates," 4th International Conference on Hydrogen Safety, San Francisco, CA, Sept. 12–14, 2011.

14. Ruggles, A.J., and Ekoto, I.W., "Ignitability and Mixing of Underexpanded Hydrogen Jets," 4th International Conference on Hydrogen Safety, San Francisco, CA, Sept. 12–14, 2011.

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16. Schefer, R., Merilo, E., Groethe, M., Houf, W., "Experimental Investigation of Hydrogen Jet Fire Mitigation by Barrier Walls," Int. Jour. of Hydrogen Energy, Vol. 36, Issue 3, pp. 2530-2537, Feb., 2011.

17. Houf, W. Evans, G., Schefer, R., Merilo, E., Groethe, M., "A Study of Barrier Walls for Mitigation of Unintended Releases of Hydrogen," Int. Jour. of Hydrogen Energy, Vol. 36, Issue 3, pp. 2520-2529, Feb., 2011.

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19. LaChance, J., Phillips, J., Houf, W., "Risk Associated with the Use of Barriers in Hydrogen Refueling Stations," National Hydrogen Association Hydrogen and Fuel Cell Safety Report, June 20, 2010.

20. Houf, W., Evans, G., Merilo, E., Groethe, M., "Evaluation of Barrier Walls for Mitigation of Unintended Releases of Hydrogen," Int. Jour. of Hydrogen Energy, Vol. 35, Issue 10, pp. 4758-4775, May 2010.

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